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13. ABSTRACT (Maximum 200 words)

The overall objective of the research program was to develop and test an improved model for the process of molecular diffusion in turbulent reactive flows. In application to turbulent combustion, a major shortcoming of existing models is that they are non-local in composition. A model has been developed, based on the construction of a Euclidean minimum spanning tree (EMST). This model is inspired by the mapping closure, and reduces to it in the case of a single composition. In general, the model is asymptotically local, and hence overcomes a major flaw in previous models. The model has been tested for decaying scalars in isotropic turbulence and for a mean scalar gradient.

Additionally, studies have been made of stochastic Lagrangian models for turbulent reactive flows; and an exact expression has been obtained for the probability density function of temperature (or other random quantities) in statistically stationary turbulence.

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1 INTRODUCTION

The treatment of molecular diffusion remains one of the major difficulties to be overcome in models of turbulent combustion. One view of the overall problem is obtained by considering how, at a given point within a turbulent combustion device, the fluid composition changes with time. There are three processes that cause this change: convection, reaction, and molecular diffusion. In pdf methods the first two of these processes are treated exactly, while the third—molecular diffusion—has to be modelled. Many other theoretical and experimental studies lead to the same conclusion: the major current issue in turbulent combustion is to understand and model the effects of molecular diffusion.

A most promising recent advance is the development of *mapping closures* (Chen et al. 1989, Kraichnan 1990, Pope 1991, Gao 1991). This is a new formalism that yields "constant-free" pdf closures. In its initial application to the marginal pdf of a scalar (Pope 1991) the accuracy of the mapping closure has been remarkable.

For simple test cases, analytic solutions to the mapping-closure equations can be obtained. But for application to inhomogeneous flows of practical importance, the closure needs to be implemented as a particle method. For a single scalar, a particle-implementation has been developed by Pope (1991). The major topic considered under the grant is the extension of these ideas to the case of multiple scalars. The resulting EMST mixing model is described in Section 2.1.

The process of molecular mixing is not, of course, independent of the velocity field that is convecting and distorting the composition fields. In pdf methods, there are separate stochastic models for the evolution of velocity and composition following fluid particles. Two papers concerning these models and their interconnection have been written and are outlined in Section 2.2.

Finally, a new *exact* result has been obtained for the pdf of *any* stationary random process, such as the temperature at a point in a turbulent combustion device. This is described in Section 2.3.

2 ACCOMPLISHMENTS

2.1 EMST Mixing Model

The term "mixing model" refers to a turbulence sub-model that describes the evolution of the pdf of composition. In the Lagrangian-pdf framework, the mixing model specifies how the composition $\boldsymbol{\phi}(t)$ evolves following a fluid particle. In one popular model (IEM) $\boldsymbol{\phi}(t)$ relaxes to the local mean value $\langle \boldsymbol{\phi} \rangle$ at a specified rate. In another class of models (particle-interaction models), the composition of the n-th particle in an ensemble $\boldsymbol{\phi}^{(n)}(t)$ changes by an exchange with another randomly selected particle (m, say, with composition $\boldsymbol{\phi}^{(m)}(t)$).

Such mixing models have been extensively examined for inert flows (e.g. Pope 1982) and several shortcomings have been identified and are now well-appreciated. More recently a different shortcoming—peculiar to reacting flows—has been identified. Specifically, the physics of the problem shows that mixing is *local in composition space* whereas the models cited above are non-local. These ideas are now explained in more detail.

In the simplest case of Fickian diffusion with uniform diffusivity Γ, the rate of change of composition $\boldsymbol{\phi}$ due to diffusion is simply $\Gamma \nabla^2 \boldsymbol{\phi}$. Since the Laplacian is a local operator, one can think of $\boldsymbol{\phi}$ changing as a result of composition differences in an infinitesimal neighborhood of the point in physical space ($\mathbf{x}$). And since the composition field is mathematically smooth, the compositions $\boldsymbol{\phi}$ at points in this neighborhood differ infinitesimally. Thus mixing is local in both physical and composition spaces. In both of the models mentioned above, the composition $\boldsymbol{\phi}^{(n)}(t)$ is influenced non-locally, either by $\langle \boldsymbol{\phi} \rangle$ or by $\boldsymbol{\phi}^{(m)}(t)$.

The EMST mixing model, now described, is an asymptotically local model, inspired by the mapping closure. For a single composition ϕ it reduces exactly to the amplitude mapping closure.

Consider first a single scalar $\phi(\mathbf{x}, t)$ in homogeneous turbulence. In a particle method, the pdf of ϕ is represented by an ensemble of N particles, the n-th having the scalar value $\phi^{(n)}(t)$.

For this problem, the mapping closure yields a fascinating particle method (Pope 1991). Let the particles be ordered so that

$$\phi^{(1)}(t) \leq \phi^{(2)}(t) \leq \ldots \leq \phi^{(N)}(t). \tag{1}$$

Then (according to the mapping closure) the particles evolve by a coupled set of ode's

$$\frac{d}{dt}\phi^{(n)}(t) = B_{n+\frac{1}{2}}\left[\phi^{(n+1)} - \phi^{(n)}\right] + B_{n-\frac{1}{2}}\left[\phi^{(n-1)} - \phi^{(n)}\right], \tag{2}$$

where (for large N) the positive coefficients are

$$B_{n+\frac{1}{2}} = N^2 A\left(\frac{n+\frac{1}{2}}{N}\right), \tag{3}$$

and A is a known function. (The coefficients $B_{\frac{1}{2}}$ and $B_{N+\frac{1}{2}}$ are zero, so $\phi^{(0)}$ and $\phi^{(N+1)}$ can remain undefined.) A simple interpretation of Eq. (2) is that $\phi^{(n)}(t)$ is drawn to its two neighbors at a rate proportional to its separation from them. Note that as N tends to infinity, the difference between $\phi^{(n)}$ and $\phi^{(n\pm1)}$ tends to zero. Hence the method is (asymptotically) local.

Consider now the general case in which there are σ compositions: in a typical combustion problem (employing simplified kinetics) σ may be 5. Then the composition for the n-th particle is denoted by

$$\phi^{(n)}(t) = \{\phi_1^{(n)}(t), \phi_2^{(n)}(t), \ldots, \sigma_\sigma^{(n)}(t)\}, \tag{4}$$

and it can be regarded as a point in the σ-dimensional composition space. Thus the ensemble of N particles correspond to N points in σ-space.

The concept of ordering—as used in Eq. (1)—is peculiar to one-space. There is no direct equivalent in multi-dimensional spaces, and so a direct extension of the model defined by Eq. (2) is not possible.

However, we have developed a model, inspired by Eq. (2), which is asymptotically local, and which reduces to Eq. (2) in the one-composition case. It is based on Euclidean minimum spanning trees (EMST). An example of an EMST (for $\sigma = 2, N = 400$) is shown in Fig. 1. By definition, the EMST is the set of edges joining the points, such that all points are connected, with the $N-1$ edges chosen (out of the N^2 possibilities) so that their total length is minimal. By this construction, one or more neighbors are identified for each particle, and hence evolution equations analogous to Eq. (2) can be constructed.

This model has been implemented and tested in up to 10 dimensions. Figures 2 and 3 show results for the test case of two decaying scalars in isotropic turbulence. The variance decays correctly, and (at least while the variance is significant) the skewness and kurtosis are close to their Gaussian values of zero and three. The cumulative distribution function (Fig. 3) is acceptably close to Gaussian.

Figure 4 shows results from a more revealing test case in which there is a mean scalar gradient. In this instance, the variance (and indeed all other statistics) attains a stationary value. The results agree well with experiments and DNS, and the skewness and kurtosis are again close to Gaussian values.

Research on this model is continuing. A reactive-flow test case is being examined, and then the model will be incorporated in a Monte Carlo PDF code.

2.2 Stochastic Lagrangian Models

The mixing model described in the previous Section fits in the general framework of stochastic Lagrangian models. Such models for the velocity, composition and other properties following fluid particles can be used to effect closure of the Lagrangian and Eulerian pdf equations. Hence they comprise a pdf turbulence model applicable to turbulent reactive flows such as combustion.

During the reporting period, two substantial papers have been completed on the topic of stochastic Lagrangian models. The first, Pope (1994a), is a tutorial review of the approach. The second, Pope (1994b), explores the relationship stochastic Lagrangian models and second-moment closures.

The major findings and contributions of the latter work are now summarized. To every stochastic Lagrangian model there is a unique corresponding second-moment closure. In terms of the second-order tensor that defines a stochastic Lagrangian model, corresponding models are obtained for the pressure-rate-of-strain and the triple-velocity correlations (that appear in the Reynolds-stress equation) and for the pressure-scrambling term in the scalar flux equation. There is advantage in obtaining second-moment closures via this route, because the resulting models automatically guarantee realizability.

Some new stochastic Lagrangian models are presented that correspond (either exactly or approximately) to popular Reynolds-stress models.

2.3 Exact Expression for Stationary PDF

Central to this project, and indeed to many issues in turbulence, is the shape adopted by the pdf's of different flow properties. In turbulent combustion the importance of pdf's has been recognized for over twenty years. In the theoretical turbulence community there is now much interest in the topic, since pdf's are a natural diagnostic for intermittency.

Together with Emily Ching, we have obtained a surprisingly simple exact expression for the pdf amplitude of *any* stationary random process (Pope & Ching, 1993). Consider, for example, the temperature $T(t)$ measured as a function of time at a particular point in a turbulent reacting flow. Let $X(t)$ be the standardization of $T(t)$, i.e.

$$X(t) \equiv (T(t) - \langle T \rangle)/\sigma_T, \tag{5}$$

where $\langle T \rangle$ and σ_T are the mean and standard deviation of $T(t)$. The result we have obtained for $P(x)$, the pdf of X, is

$$P(x) = \frac{C_1}{\langle \dot{X}^2 | x \rangle} \exp\left\{ \int_0^x \frac{\langle \ddot{X} | x' \rangle}{\langle \dot{X}^2 | x' \rangle} dx' \right\}, \tag{6}$$

where C_1 is a normalization constant, and $\langle \ddot{X} | x \rangle$ denotes the expectation of the second time derivative of $X(t)$ conditional on $X(t) = x$.

In experiments, simulations and modelling, this formula provides a valuable connection between the pdf and the time derivatives of the signal. As discussed by Pope & Ching (1993) it sheds light on the tail-shape of pdf's, and it explains the success of a previous empirical expression due to Ching.

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Pope, S.B. (1994a) Annu. Rev. Mech. **26**, 23.

Pope, S.B. and Ching, E.S.C. (1993) Phys. Fluids A **5**, 1529.

4 PUBLICATIONS

During the reporting period, the following papers acknowledging support from this grant have been published:

S.B. Pope (1994) "Lagrangian PDF Methods for Turbulence," Annual Reviews of Fluid Mechanics, Vol. **26**, 23–63.

S.B. Pope and E.S.C. Ching (1993) "Stationary probability density functions in turbulence," Physics of Fluids A **5**, 1529–31.

S.B. Pope (1994) "On the relationship between stochastic Lagrangian models of turbulence and second-moment closures," Physics of Fluids **6**, 973–985.

Subramanian, S. and Pope, S.B. (1992) "Limitations of the Amplitude Mapping Closure," Bull. Am. Phys. Soc. **37**, 1805.

5 PERSONNEL

The following personnel have received support from the grant.

Professor S.B. Pope, PI

Tom Dreeben, Ph.D. Student

Shankar Subramanian, Ph.D. Student

Dr. Song Fu, Post-doc.

6 INTERACTIONS

During the reporting period, the PI has had significant technical interactions with:

General Electric, Corporate Research & Development

General Electric, Power Generation

Allison Engine Company

University of Stuttgart

University of Sydney

NASA Langley

Stanford/Ames Center for Turbulence Research

7 INVENTIONS AND PATENTS

None.

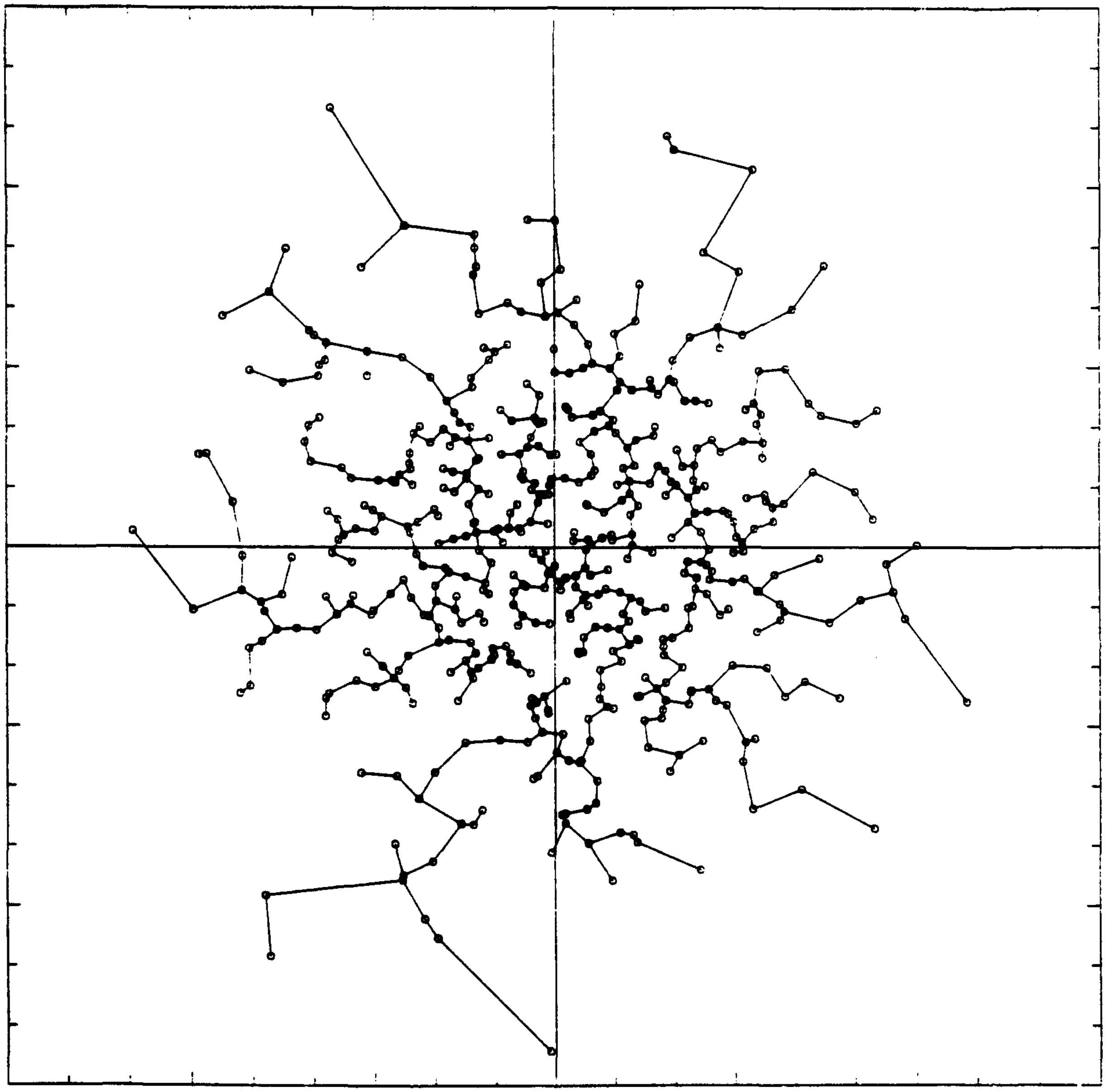

Fig. 1: A Euclidean Minimum Spanning Tree (EMST) in two dimensions.

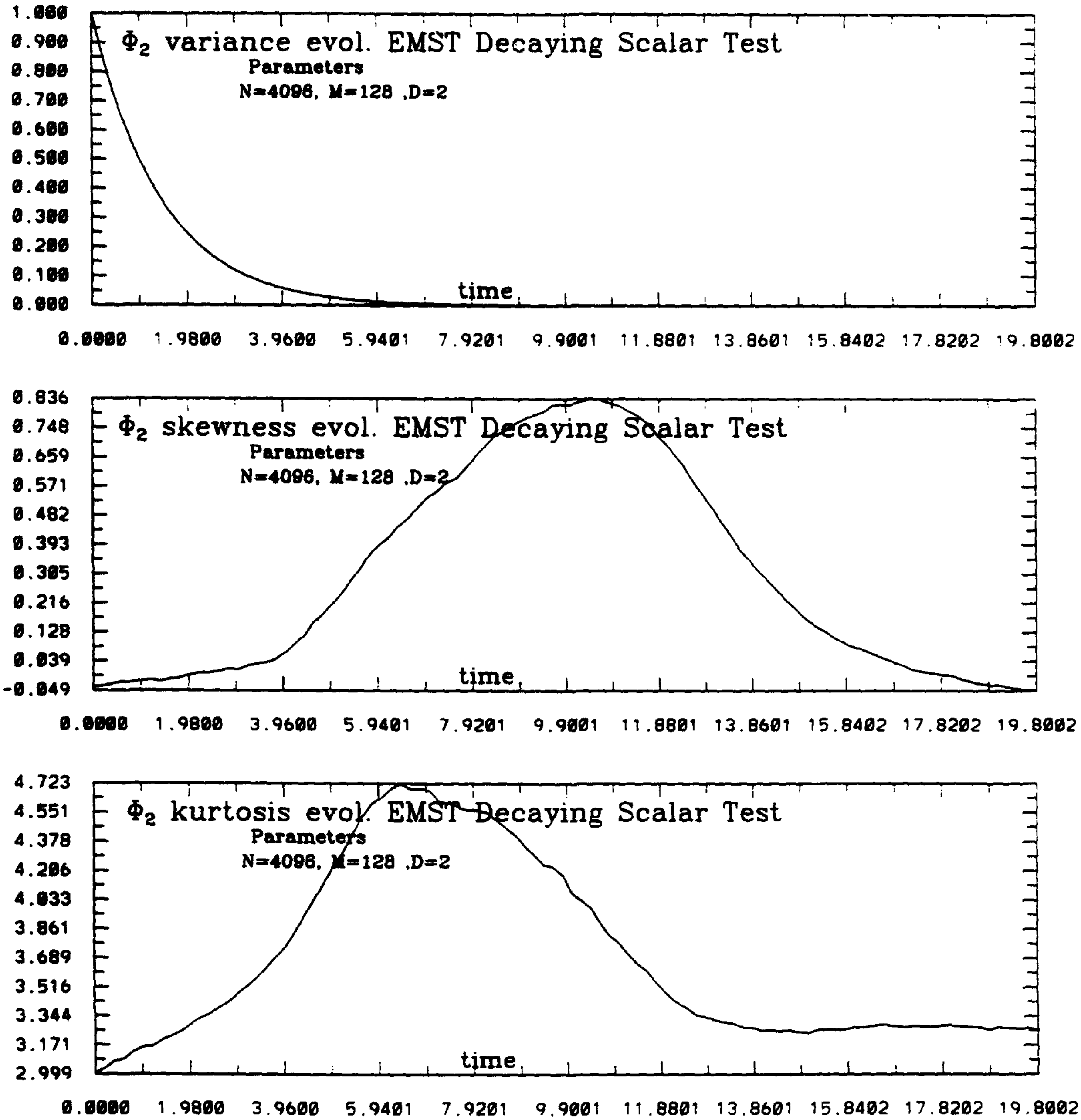

Fig. 2: EMST mixing model applied to two decaying scalars in isotropic turbulence. Temporal evolution of a) the variance b) the skewness and c) the kurtosis of one scalar.

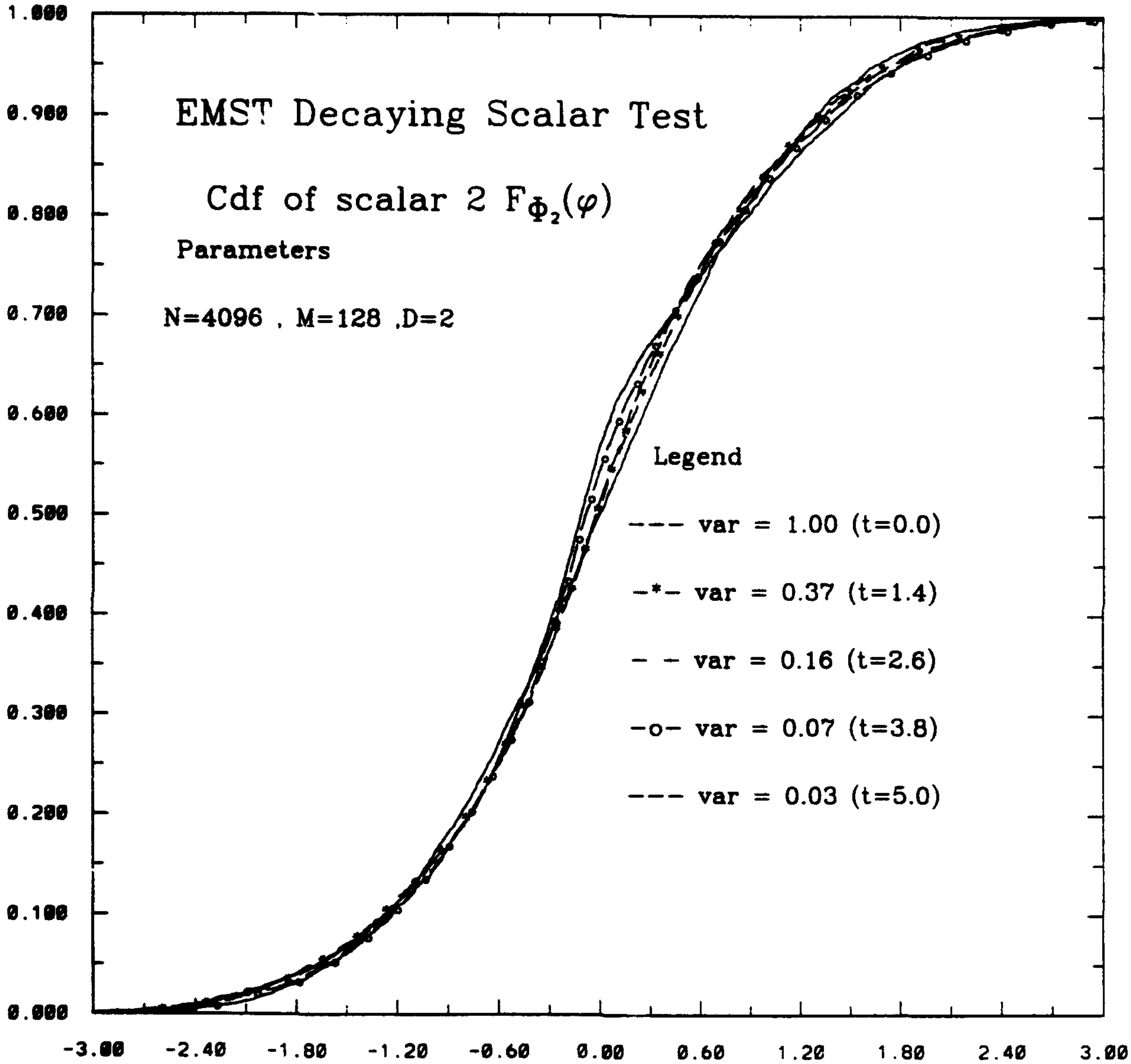

Fig. 3: EMST mixing model applied to two decaying scalars in isotropic turbulence. Cumulative distribution functions of standardized scalar at different times, showing that the scalar remains close to Gaussian (as it is at $t = 0$).

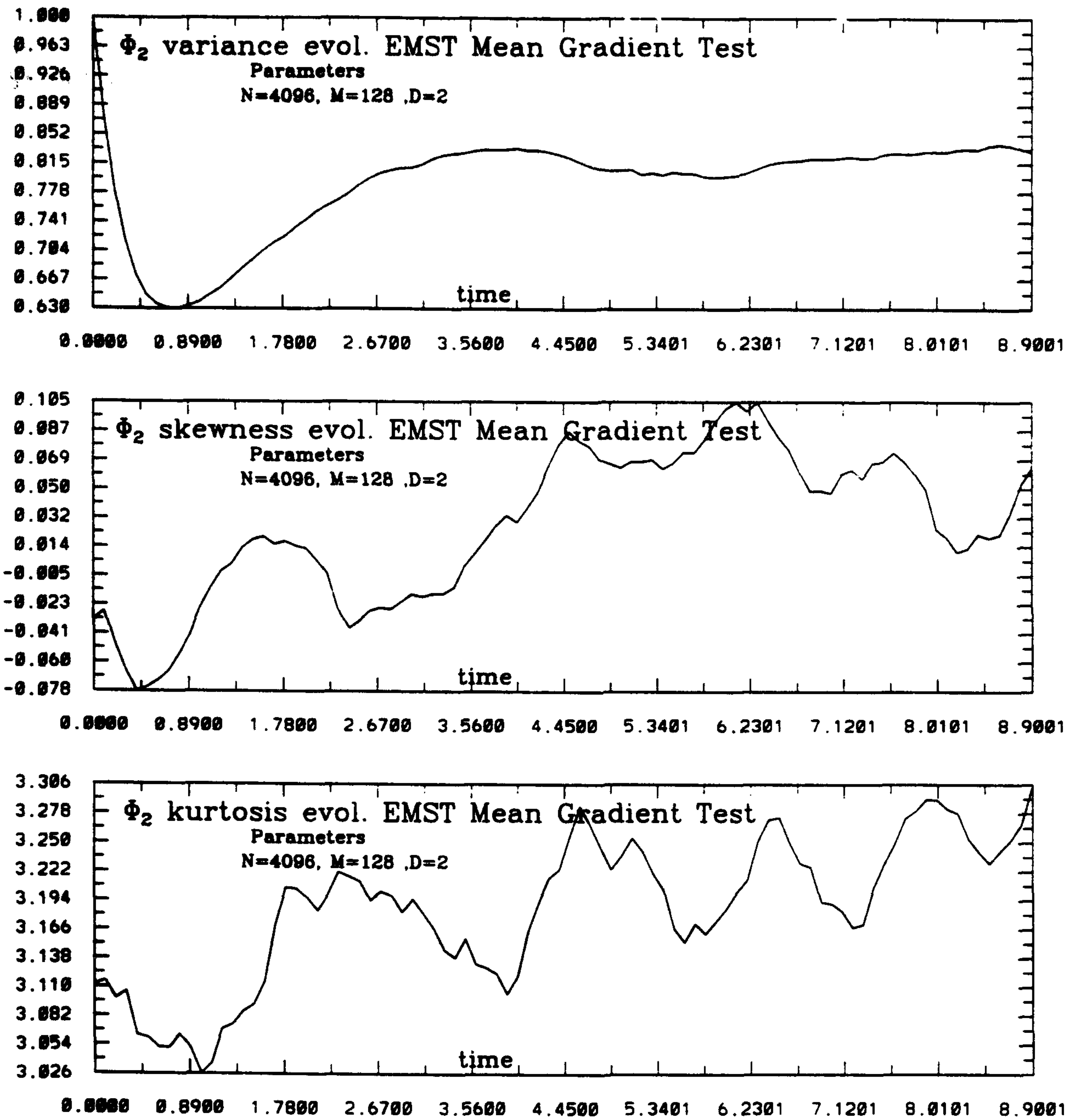

Fig. 4: EMST applied to two scalars with uniform mean gradients in isotropic turbulence. Temporal evolution of a) the variance b) the skewness and c) the kurtosis for one of the scalars.